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3D numerical simulations as optimization tool for the design of novel EMAP systems

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ABSTRACT

An innovative biodegradable bio-based packaging system has been designed to achieve Equilibrium Modified Atmosphere Packaging (EMAP) of high value fresh horticultural produce through optimised barrier properties obtained by laser micro-perforations combined with selectively permeable membrane technologies. Polylactic Acid (PLA) film was used as packaging material replacing conventional biaxial oriented polypropylene (BOPP) films. The tested commodities were fresh cherry tomatoes and peaches. The micro-perforated PLA EMAP packages appear to perform very well for both commodities due to their higher water vapour permeability compared to conventional materials. 3D numerical simulations were employed as a tool to design and analyse the performance of the novel EMAP system. The numerical simulations results were found to be in good agreement with the experimental data, with the average values differences being within the standard deviations ($< 5\%$). The numerical results were also found to agree with the average values predicted by an analytical model. The computational analysis provided detailed 3D mapping of the gas mixture concentrations in the EMAP headspace. 3D mapping not only confirmed the experimental average data but also identified dysfunctional packaging details and explained fruit skin deformations and regions of water vapour condensation observed in conventional BOPP EMAP.

1. Introduction

The development of thin transparent barrier films offered new possibilities to the food packaging industry. Packing food in equilibrium modified atmosphere (EMAP) is a method for prolonging the shelf life of fresh horticultural produce by controlling the in-package equilibrium atmosphere (Del-Valle et al., 2009). This can be achieved by modifying the permeability of the conventional packaging film through perforations or micro-perforations, in order to regulate the equilibrium concentrations of O_2, CO_2 and relative humidity RH.

Various approaches have been proposed to model gas transfer through perforated films of food packages (Chung et al., 2003; Gonzalez et al., 2008). Most models are based on Fick's law of diffusion (Chung et al., 2003) or Stefan–Maxwell law (Rennie and Tavoularis, 2009a,b). An end correction term is introduced in these models for the diffusive path length of the perforations to compensate for end effects at the perforation mouths (Chung et al., 2003). No such corrections are needed when 3D computer simulations are applied for modeling diffusion through a perforation.

Previous research works on EMAP created mathematical models in order to describe the physiological and gas transport processes (Melkikh and Seleznev, 1994; Fishman et al., 1995; Fishman et al., 1996; Fonseca et al., 2000; Paul and Clarke, 2002). In most of these studies simplified analytical methods were applied. Computational simulations of gas diffusion for modeling EMA in packaging of fresh fruit and vegetables are limited in literature (Rennie and Tavoularis, 2009b; De Bonis et al., 2015). Numerical simulations could be employed to model in detail the headspace gas composition distribution around the packaged products and guide the design and the key parameters optimisation of EMA packages, complemented and confirmed by laboratory tests.

Environmental concerns recently press towards a change in the materials used in the agrifood industry, including food packaging materials, from conventional fossil-based plastics to biodegradable plastics made of sustainable resources (Picuno, 2014). Various bio-based polymers, such as Polylactic Acid (PLA from now on) and starch based plastics have been evaluated as packaging materials despite their current relatively higher cost (Auras et al., 2004). Such new materials have different gas permeability properties as compared to conventional plastics (Curtzwiler et al., 2008).

Biaxial Oriented Polypropylene (BOPP) is among the favored commercial packaging materials in the market and suitable for the food

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packaging industry. The barrier properties of BOPP differ from those of bio-based films such as PLA mainly with respect to its Water Vapour (WV from now on) permeability that is much lower than the transpiration rate of the studied produce. BOPP film is practically considered impermeable to water vapor. This means that the exchange of all the gases of the mixture in the package headspace (CO_2, O_2 and WV) with the environment can only occur through perforations. Most commercial BOPP food packages have macro-perforations (i.e. large-size perforations). As a result the CO_2 concentration in the package is similar to the atmospheric value.

PLA is a bio-based polymer, compostable under industrial composting conditions. Bio-based films such as PLA have been successfully tested for specific food packaging purposes. Usually, bio-based films, including PLA, have water vapour transmission rates (WVTR) much higher than the conventional BOPP films. In the case of perforated bio-based packaging systems, the effect of the perforations on water vapour permeability is influenced by the permeability of the film to WV. In the work of Mistriotis et al. (2011) it was shown that the effect of a perforation on WV permeability decreases as the WVTR of the film increases. On the other hand, the same bio-based films behave as barriers with respect to CO_2 and O_2 with similar transmission rates to BOPP films. This versatility of bio-based biodegradable or compostable materials offers new possibilities in optimizing the design of EMAP systems for fresh horticultural products while it allows for an environmentally friendly disposal of the packaging waste.

The aim of this work was to analyze the performance of bio-based EMAP systems for two important commercially European horticultural products, cherry tomatoes and peaches, by 3D numerical simulations. The specific fresh products were chosen because they are typical representatives of the two main categories of fresh produce, namely vegetables (or small fruits) and fruits (or large fruits). They were selected for their commercial importance, high value, and sensitivity. The postharvest management of these fresh produce includes packaging using various alternative packaging systems, transportation, storage, and trading (retailers, exported-imported). The analytical model of Mistriotis et al. (2016) was used to design innovative PLA based EMAP systems for the selected fresh products. The aim of the innovative EMAP design was to ensure good quality, safety and longer shelf life of the fresh produce while eliminating the use of fossil-based commercial packaging materials.

The performance of micro-perforated PLA EMA packages with cherry tomatoes and peaches were tested in the laboratory. For comparison purposes unpacked, macro-perforated BOPP EMA packages were also tested. The results of the experimental investigation of the innovative EMAP design were presented in Briassoulis et al. (2013). The unpacked products showed very early significant loss of water. The macro-perforated BOPP packages failed to regulate the WV exchange between the package and the environment. For the cherry tomatoes case early skin deformations were detected (shrinkage), while for the peaches WV condensation was observed on the interior surface of the package envelope, which is associated to rapid infections development. The products packed in the PLA based EMAP systems were shown to be of high quality for a longer shelf life-time.

The paper presents a numerical simulation methodology that is used as a design and analysis tool for the evaluation of fresh produce EMAP configurations. The method is used to perform design optimization of the EMAP solutions proposed by an analytical model (Mistriotis et al., 2016) (i.e. refining the envelope area and micro-perforations on the packaging film), and to analyze the performance of EMAP of fresh produce tested under laboratory controlled conditions (Briassoulis et al., 2013).

2. Materials and methods

2.1. Basic definitions

The terminology used is briefly presented in this section for the convenience of the reader. A more detailed presentation can be found in Mistriotis et al. (2016) The one dimensional diffusion of a gas through a permeable film or a membrane can be described by Fick's law (e.g. Versteeg and Malalasekera, 1995):

$$F= PA\frac{dp}{dx} \tag{1}$$

F, the diffusion flow rate through the film, can be expressed in two different ways: the volume flow rate F ($m^3\ s^{-1}$) or the mass flow rate F ($kg\ s^{-1}$)

dp/dx ($Pa\ m^{-1}$) is the gas pressure gradient across the specimen

A (m^2) is the area of the film

P is the gas permeability of a material and at constant temperature and is expressed as gas mass permeability P ($kg\ m\ m^{-2}\ s^{-1}\ Pa^{-1}$) or gas volume permeability P ($m^3\ m\ m^{-2}\ s^{-1}\ Pa^{-1}$).

A different expression of Fick's law equation (Eq. (2)) can be provided if the partial pressure gradient is replaced by the molar fraction gradient of the gas, dc/dx (m^{-1}).

$$F= PA\frac{dc}{dx} \tag{2}$$

In this expression, gas permeability P is measured in ($kg\ m\ m^{-2}\ s^{-1}$, mass permeability) or in ($m^3\ m\ m^{-2}\ s^{-1}$, volume permeability).

The one dimensional diffusion of a gas in a gas mixture is described by Eq. (3). Eq. (3) provides similarly to Eq. (2) the gas diffusion volume flow rate F, but the gas volume permeability, P ($m^2\ s^{-1}$), is now substituted by diffusion coefficient or kinematic diffusivity D ($m^3\ m\ m^{-2}\ s^{-1}$) or equally D ($m^2\ s^{-1}$) (Note: it is implied that analogous definitions apply to gas diffusion mass flow rate related quantities):

$$F = DA\frac{dc}{dx} \tag{3}$$

The transmission rate TR of a gas mass ($kg\ m^{-2}\ s^{-1}$) or volume ($m^3\ m^{-2}\ s^{-1}$) through a membrane is given by Eq. (4):

$$TR = \frac{F}{A} \tag{4}$$

The transmission rate (TR) is defined as the gas flux (flow rate per area unit F/A). Where, F ($kg\ s^{-1}$) or ($m^3\ s^{-1}$) is the gas mass or volume flow rate.

Eq. (5) presents a modification of Fick's law applicable to the diffusion of gases through a single perforation:

$$F_D = DA_P\frac{\Delta c}{L+ kd} \tag{5}$$

In this case, F_D ($m^3\ s^{-1}$) is the gas diffusion volume flow rate through a hole, D ($m^2\ s^{-1}$) is the diffusion coefficient of the considered gas in air, L (m) is the thickness of the film, Δc is the molar fraction difference of the gas across the hole, A_P (m^2) is the area of the perforation, d (m) is the perforation diameter and k is a phenomenological factor describing the end effects of the perforation (Chung et al., 2003). The diffusion through a perforation is modelled as diffusion through a finite tube, modified to incorporate end effects at the perforation's mouths. End effects become significant when perforations have low L/d aspect ratios (Chung et al., 2003).

Typical k factor values (Eq. (5)), representative of perforations' end effects vary in the range 0.4–1.0 (Gonzalez et al., 2008). For the extreme value of $k = 0$ this empirical law corresponds to Fick's law (i.e. no end effects).

2.2. Methodology

A numerical simulation methodology is developed and used as a complementary design tool for the optimization of EMA Package